

Joint Research Centre

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Technology portfolio

METIS - Metabolic Information Input System

Description

The assessment of chemical reactivity and metabolism is an important aspect in the risk assessment of chemicals and should be assisted by the application of computational tools. METIS (Metabolic Information Input System) is a user-friendly open source application designed for the storage and input of information on metabolism and degradation reactions. The resulting database is compatible with the CRAFT software tool (which stimulates chemical and metabolic reactions) but has also been designed to exchange reaction data with other software tools.

Innovative aspects and main advantages

- ▶ Standalone tool that allows chemical reactions and metabolic pathways to be drawn, edited, manipulated and annotated.
- ▶ Annotation of the reactions and pathways with additional information.
- ▶ To complement the reaction information, atom-atom mappings may be assigned to the reactions as well.
- ▶ Graphical input of metabolic pathways and degradation reactions into a database (MySQL) by a convenient and easy-to-use GUI.

Areas of application

- ▶ EU agencies (particularly ECHA, EFSA and EEA)
- ▶ Industry
- ▶ Academic research

Maturity and availability

- ▶ Mature product (available under EUPL licence version 1.1)
- ▶ Open-source and freely available software package available for download from both the JRC and the Molecular Networks web sites.
- ▶ Typically, METIS is used as a supplement to CRAFT applications. CRAFT can be obtained both from the JRC and Molecular Networks web sites.
- ▶ In order to be able to use METIS on a stand-alone dedicated computer it is necessary to have the MySQL server installed. Available for download at: www.mysql.com

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Licensing contact

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